Silvia Chellini

Project Promoter

Reference Network in Theoretical and Computational Chemistry

http://www.xrqtc.com

Bilateral Meetings

- Friday (9:00am - 12:00pm)
- Friday (12:00pm - 4:00pm)

Description

The XRQTC is a public entity which coordinates research groups in computational chemistry, helping to promote their works, expertise and knowledge. It helps and encourage the research valorization by the transfer of the technologies to the society, both public or private sector. Otherwise it promotes scientific training high-level activities in the field of theoretical and computational chemistry, such as seminars, workshops and conferences.

The Network is a pioneer in the use of computational methods to research the properties of solid inorganic materials and molecular materials of technological interest, and of surfaces and nanostructures. We design and optimise catalysts and nanocatalysts for the improvement of industrial processes. We use simulation to evaluate and predict the creation of new materials and nanomaterials, polymers and synthetic materials.

We develops bio- and cheminformatics tools for the discovery of new active compounds in drug design using methods of docking, molecular modelling and hybrid methods of quantum and classical mechanics. We simulate processes of enzyme catalysis for the design of new stable enzymes, for applications in biotechnology, biomedicine and industrial processes.

The Network contributes to research in atmospheric pollution using theoretical chemistry and simulation tools, applied to the dynamics of chemical reactions. We study how to optimise processes of selective adsorption of industrial gases on solid and liquid materials with a view to improving their uptake and reducing global emissions. We study the physiological properties and environmental toxicity of chemical, organic and nanomaterial substances.

For more information, please visit: www.xrqtc.com

Organization Type

University

Founding Year

2007

Phone

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Country

Spain

City
Barcelona08028, c/baldiri reixac 4-8 Google map
Offer

Crystal Engineering

We have developed an efficient tool able to predict polymorphs for crystals of pharmacological, based on a semi-empirical approach and a low computational cost numerical method.

We offer a consulting service to laboratories and manufacturers interested in performing crystal optimizations and polymorph predictions.

Keywords: polymorphs crystal engineering APIs
Cooperation Offered

1. Technical co-operation
2. Outsourcing co-operation

Offer

Analysis of biological systems

We carry out interdisciplinary research, combining own biochemistry techniques, cell and molecular biology and bioinformatics for the integrated analysis of biological systems.

We offer the following services:

• Fluxomic and metabolomic analysis of biological samples.
• Assessment of biological activity of new compounds with anti-tumor activity.
• Trials in-vivo animal models.
• Modeling of biochemical systems.
• Evaluation of natural products: characterization of potential derived from natural products and by-products as high value-added products.

Keywords: Metabolomic Natural products functional food
Cooperation Offered

1. Technical co-operation
2. License agreement

Cooperation Requested

1. Technical co-operation

Offer

Computer aided drug design

We work in different early stage drug discovery processes, using several computational methodologies, which can help your project move forward.

We develop different tasks in the following stages:

Target Identification & Validation

Library Design

Hit Identification

Lead Optimization

Drug Repurposing

Keywords: drug discovery computer aided drug design BIOINFORMATICS CHEMOINFORMATICS
Cooperation Offered

1. Technical co-operation
2. Outsourcing co-operation

Offer

Design of enzymes and inhibitors

We apply the biomolecular simulation to the enzyme engineering with the aim of showing how the activity/function of biomolecules can be regulated or modified using inhibitors, allosteric effects, mutations or radiation, or a combination of them.

We also develop a computational protocol to routinely design enzymes useful for any chemical reaction of pharmaceutical interest.

Keywords: enzyme engineering biomolecular simulation
Cooperation Offered

1. Technical co-operation

Cooperation Requested

1. Outsourcing co-operation
2. Technical co-operation

Offer

Computational tools for industrial application

The Xrqtc coordinates research groups experts in material science, life and food science, environmental.
We offer solutions for chemical, pharmaceutical, cosmetic and food industry.

We are looking for partners or consortia to participate in H2020 calls, having large experience in participating in different types of projects.

High interesting topics:

SC1-PM-16-2017: In-silico trials for developing and assessing biomedical products
SC1-PM-17-2017: Personalised computer models and in-silico systems for well-being

Keywords: #computationalchemistry #drugdesign #enzymcatalysis
Cooperation Offered

1. Technical co-operation

Cooperation Requested

1. Outsourcing co-operation
2. Technical co-operation